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6. AUTHOR(S)
James G. Brasseur

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
The Pennsylvania State University, Department of Mechanical Engineering, 123 Reber Buiding, University Park, PA 16802

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13. ABSTRACT (Maximum 200 words)

The diffusion of passive scalar pollutants in the atmosphere can constitute serious environment hazards. Recent studies have pointed to the increased danger associated with extremely high instantaneous point concentrations. We analyzed the local turbulence structure underlying statistical descriptions of turbulent diffusion. Specifically, we analyzed the entrainment of passive scalar across a buoyancy-driven convective boundary layer (CBL) capping inversion using 963 and 1283 large-eddy simulation (LES). In the simulations, a uniform concentration of passive scalar was released in the stable layer above a CBL with a strong capping inversion (963 LES) and a CBL with a weak capping inversion (1283 LES). The local turbulence structure in and around the entrainment layers were analyzed using graphical imaging, single-point statistical measures and conditional statistics. Among other things we found that We found the entrainment of top-down passive scalar to be more rapid with the weaker capping inversion suggesting that entrainment from above is affected by boundary layer growth, and that entrainment was concentrated in low vorticity downdraft regions which transport scalar directly through the capping inversion.

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Applications of New Concepts in Scientific Analysis to Atmospheric Studies

Statement of problem studied

The diffusion of passive scalar pollutants in the atmosphere can constitute serious environment hazards. Recent studies have pointed to the increased danger associated with extremely high instantaneous point concentrations. We analyzed the local turbulence structure underlying statistical descriptions of turbulent diffusion. Specifically, we analyzed the entrainment of passive scalar across a buoyancy-driven convective boundary layer (CBL) capping inversion using 96^3 and 128^3 large-eddy simulation (LES). In the simulations, a uniform concentration of passive scalar was released in the stable layer above a CBL with a strong capping inversion (96^3 LES) and a CBL with a weak capping inversion (128^3 LES). The local turbulence structure in and around the entrainment layers were analyzed using graphical imaging, single-point statistical measures and conditional statistics.

Summary of most important results

We found the entrainment of top-down passive scalar to be more rapid with the weaker capping inversion suggesting that entrainment from above is affected by boundary layer growth. Locally, scalar penetration in the mixed layer was strongly influenced by the initial horizontal distribution of updrafts and downdrafts at the time of scalar release. The local dynamics of entrainment changed, however, after an initial period of high scalar flux lasting approximately one large-eddy turnover time. Entrainment then entered a quasi-steady asymptotic period with different entrainment behavior.

During the initial period, the local scalar flux in the immediate vicinity surrounding penetrative updrafts was negative and resulted form the turning motions of rising fluid downward. In the asymptotic state, by contrast, relatively little scalar entered the CBL in the immediate vicinity where the plumes were redirected downward by the capping inversion. Rather, most of the negative flux regions which contained positive scalar fluctuations coincided with downdrafts driven by the Rayleigh-Bénard cellular structures in the mixed layer. These far region downdrafts were the primary source of transport of scalar from above the capping inversion, they persisted independently of variations in the strength of neighboring updrafts, and they were the primary pathways for scalar entrainment. Localized mixing associated with large-horizontal-scale resolved vorticity to a large extend determined the local structure of positive scalar fluctuations found in these pathways, and this vorticity field appeared to determine the change in local structure of entrainment during the initial transition to the quasi-steady asymptotic entrainment state.

The description of a well-defined "entrainment layer" of smaller-scale eddies which transport scalar from above to below the mixed layer was not consistent with what was observed from the large-eddy simulations. Instead, entrainment was found to be concentrated in low vorticity downdraft regions which transport scalar directly through the capping inversion. Once the scalar was transported into the mixed layer, it was dispersed by local mixing processes. We find that top-down scalar diffusion is strongly influenced by the local structure of the mixed layer velocity and vorticity fields. The local velocity and vorticity structure appeared to determine the concentration levels and structure of the more intense positive scalar fluctuations within the mixed layer.

List of publications and technical reports

Cotter, John J. 1997 *Scalar Entrainment through the Capping Inversion of the Atmospheric Boundary Layer.* M.S. Thesis, Department of Mechanical Engineering, The Pennsylvania State University, University Park, PA.

Cotter, J.J., Brasseur, J.G., Khanna, S., Wyngaard, J.C. 1996 Scalar entrainment through the capping inversioin of the atmospheric boundary layer. (abstract) *Bull. Amer. Phys. Soc.* **41**(9): 1821

List of participating scientific personnel

John. C. Cotter III, M.S. student (supported on this grant)

Samir Khanna, Ph.D. student (supported on a related grant)

Brian Moquin, M.S. student (supported for 1 year on this grant)

John. C. Wyngaard, co-investigator with related grant

James G.Brasseur, pinciple investigator

Report on inventions

None.